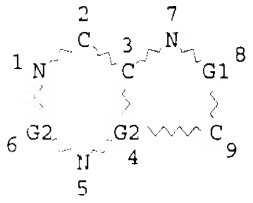
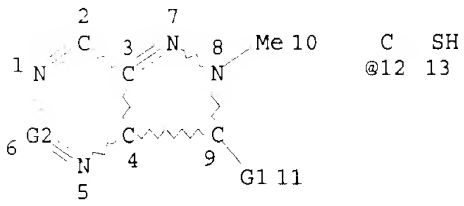
Structure box

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 08:32:49 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   17 SEP 2002  HIGHEST RN 452274-20-3
DICTIONARY FILE UPDATES:  17 SEP 2002  HIGHEST RN 452274-20-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d his

     (FILE 'REGISTRY' ENTERED AT 08:29:52 ON 19 SEP 2002)
                DEL HIS Y

     FILE 'REGISTRY' ENTERED AT 08:32:36 ON 19 SEP 2002
                ACT SIXA/A
                ---------
L1                STR
L2   (       6184)SEA FILE=REGISTRY SSS FUL L1
L3                STR
L4             18 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
                  ---------


=> d que stat
L1                STR
```




```
VAR G1=C/N/O/S
VAR G2=C/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   9
```

STEREO ATTRIBUTES: NONE
L2 (6184) SEA FILE=REGISTRY SSS FUL L1
L3 STR



VAR G1=AK/CY
VAR G2=CH/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 13

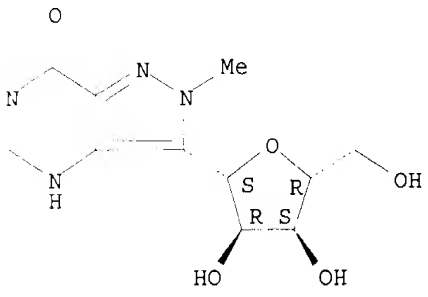
STEREO ATTRIBUTES: NONE
L4 18 SEA FILE=REGISTRY SUB=L2 SSS FUL L3

100.0% PROCESSED 3002 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.02

=> d ide can l4 1-18

L4 ANSWER 1 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 96221-17-9 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl-, monohydrochloride (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H14 N4 O5 . Cl H
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (51481-59-5)

Absolute stereochemistry.

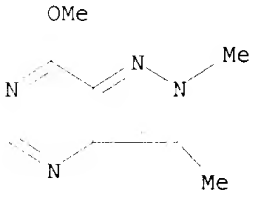


● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 102:185417

L4 ANSWER 2 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 91225-97-7 REGISTRY
CN 2H-Pyrazolo[4,3-d]pyrimidine, 7-methoxy-2,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C8 H10 N4 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



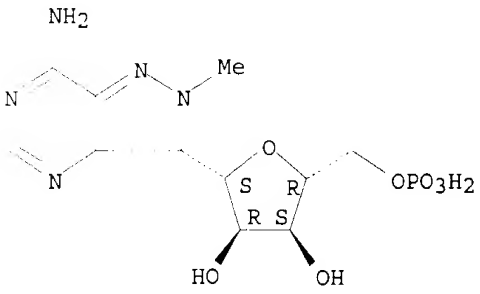
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 101:72691

L4 ANSWER 3 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 91034-38-7 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 5-(dihydrogen phosphate), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C11 H16 N5 O7 P
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



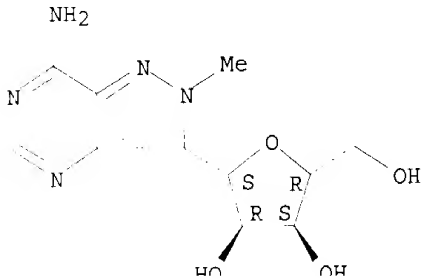
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 101:50520

L4 ANSWER 4 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 82538-44-1 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, conjugate monoacid, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C11 H15 N5 O4 . H
LC STN Files: CA, CAPLUS
CRN (42204-46-6)

Absolute stereochemistry.

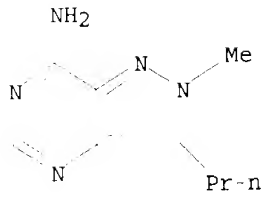


● H^+

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:72675

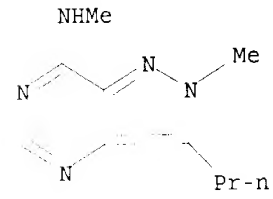
L4 ANSWER 5 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 82538-43-0 REGISTRY
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2-methyl-3-propyl-, conjugate monoacid (9CI) (CA INDEX NAME)
MF C9 H13 N5 . H
LC STN Files: CA, CAPLUS
CRN (76424-71-0)



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:72675

L4 ANSWER 6 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 76424-80-1 REGISTRY
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, N,2-dimethyl-3-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H15 N5
LC STN Files: CA, CAPLUS

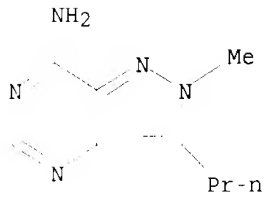


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 94:65608

L4 ANSWER 7 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 76424-71-0 REGISTRY
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2-methyl-3-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H13 N5
CI COM
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

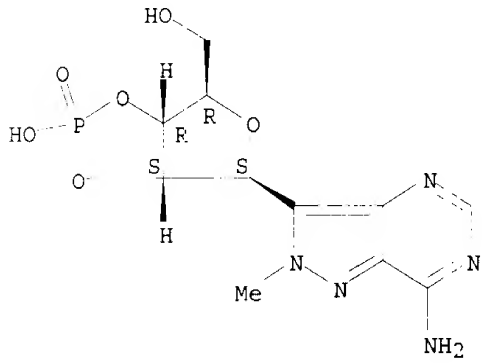
REFERENCE 1: 98:139399

REFERENCE 2: 97:72675

REFERENCE 3: 94:65608

L4 ANSWER 8 OF 18 REGISTRY COPYRIGHT 2002 ACS
PN 67187-24-0 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 2,3-(hydrogen phosphate), monoammonium salt, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
CN Furo[3,4-d]-1,3,2-dioxaphosphole, D-ribitol deriv.
FS STEREOSEARCH
MF C11 H14 N5 O6 P . H3 N
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



● NH_3

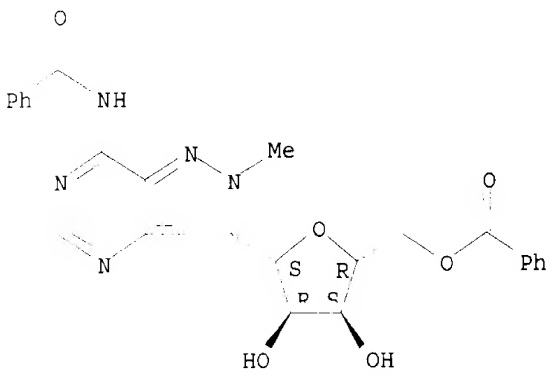
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44084

L4 ANSWER 9 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 67187-23-9 REGISTRY
CN Benzamide, N-[3-(5-O-benzoyl-.beta.-D-ribofuranosyl)-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, benzamide deriv.
FS STEREOSEARCH
MF C25 H23 N5 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



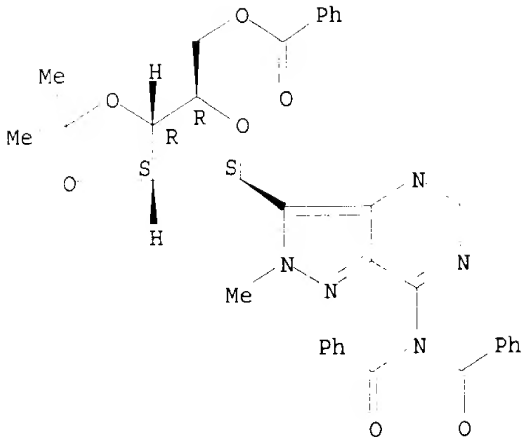
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44084

L4 ANSWER 10 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 67187-22-8 REGISTRY
CN Benzamide, N-benzoyl-N-[3-[5-O-benzoyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranosyl]-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, benzamide deriv.
CN Furo[3,4-d]-1,3-dioxole, benzamide deriv.
FS STEREOSEARCH
MF C35 H31 N5 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



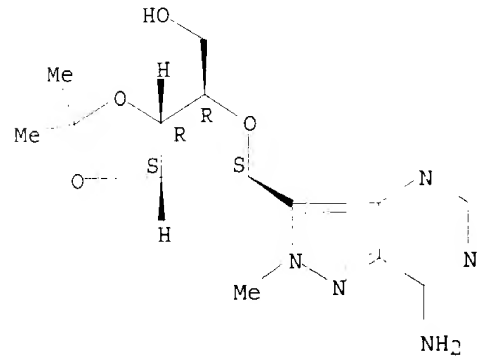
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44084

L4 ANSWER 11 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 67187-21-7 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-2,3-O-(1-methylethylidene)-, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
CN Furo[3,4-d]-1,3-dioxole, D-ribitol deriv.
FS STEREOSEARCH
MF C14 H19 N5 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

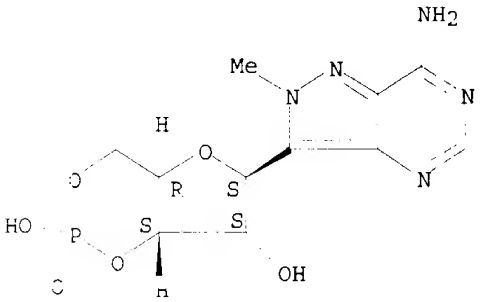
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44084

L4 ANSWER 12 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 67187-18-2 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
CN 4H-Furo[3,2-d]-1,3,2-dioxaphosphorin, D-ribitol deriv.
FS STEREOSEARCH
MF C11 H14 N5 O6 P
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



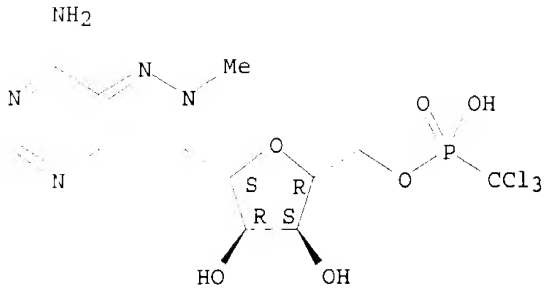
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 91:211773

REFERENCE 2: 89:44084

L4 ANSWER 13 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 67187-17-1 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 5-[hydrogen (trichloromethyl)phosphonate], hydrochloride (2:1), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C12 H15 Cl3 N5 O6 P . 1/2 Cl H
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



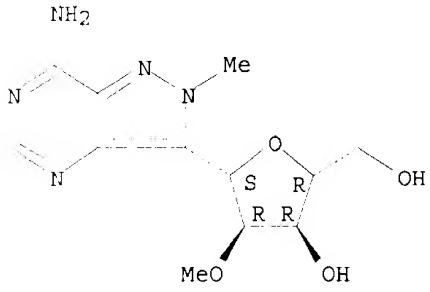
●1/2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:44084

L4 ANSWER 14 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 65300-27-8 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-2-O-methyl-, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C12 H17 N5 O4
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

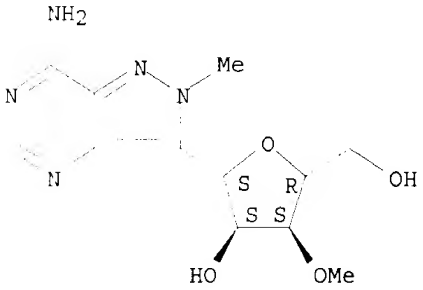
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 88:38100

L4 ANSWER 15 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 65300-26-7 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-3-O-methyl-, (S)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C12 H17 N5 O4
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



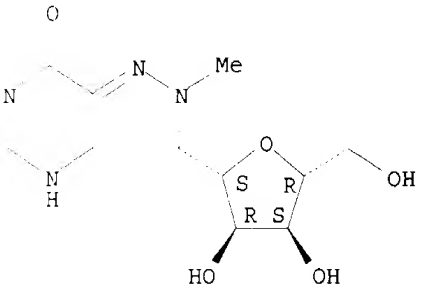
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 88:38100

L4 ANSWER 16 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 51481-59-5 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Methylformycin B
FS STEREOSEARCH
MF C11 H14 N4 O5
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1967 TO DATE)

7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:172780

REFERENCE 2: 105:54102

REFERENCE 3: 105:54101

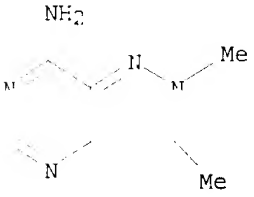
REFERENCE 4: 103:189207

REFERENCE 5: 102:185417

REFERENCE 6: 102:167081

REFERENCE 7: 81:78181

L4 ANSWER 17 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 51222-25-4 REGISTRY
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2,3-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C7 H9 N5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 98:139399

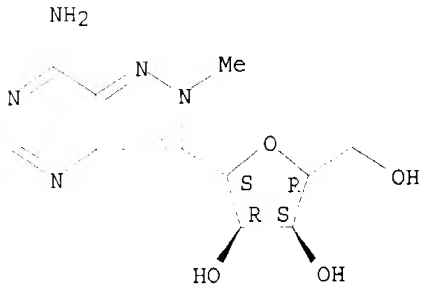
REFERENCE 2: 85:143394

REFERENCE 3: 81:78181

L4 ANSWER 18 OF 18 REGISTRY COPYRIGHT 2002 ACS
RN 42204-46-6 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)-
OTHER NAMES:
CN 2-Methylformycin
CN NSC 143684
FS STEREOSEARCH
MF C11 H15 N5 O4
CI COM

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, SPECINFO, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19 REFERENCES IN FILE CA (1967 TO DATE)
19 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:218730

REFERENCE 2: 117:43336

REFERENCE 3: 102:185417

REFERENCE 4: 102:167081

REFERENCE 5: 98:139399

REFERENCE 6: 97:72675

REFERENCE 7: 93:26714

REFERENCE 8: 92:193903

REFERENCE 9: 92:209

REFERENCE 10: 91:117147

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:36:38 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

strictly prohibited.

FILE COVERS 1907 - 19 Sep 2002 VOL 137 ISS 12
FILE LAST UPDATED: 18 Sep 2002 (20020918/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> s l4
L5 27 L4

=> d .ca hitstr l5 1-27

L5 ANSWER 1 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:793457 HCAPLUS
DOCUMENT NUMBER: 132:218730
TITLE: Formycin A and its N-methyl analogues, specific inhibitors of E. coli purine nucleoside phosphorylase (PNP): induced tautomeric shifts on binding to enzyme, and enzyme ligand fluorescence resonance energy transfer
AUTHOR(S): Kierdaszuk, B.; Modrak-Wojcik, A.; Wierzchowski, J.; Shugar, D.
CORPORATE SOURCE: Institute of Experimental Physics, Department of Biophysics, University of Warsaw, Warsaw, 02-089, Pol.
SOURCE: Biochimica et Biophysica Acta (2000), 1476(1), 109-128
CODEN: BBACAQ; ISSN: 0006-3002
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Steady-state and time-resolved emission spectroscopy were used to study the interaction of Escherichia coli purine nucleoside phosphorylase (PNP) with its specific inhibitors, viz. formycin B (FB), and formycin A (FA) and its N-methylated analogs, N(1)-methylformycin A (m1FA), N(2)-methylformycin A (M2FA) and N(6)-methylformycin A (m6FA), in the absence and presence of phosphate (Pi). Complex formation led to marked quenching of enzyme tyrosine intrinsic fluorescence, with concomitant increases in fluorescence of FA and m6FA, independently of the presence of Pi. Fluorescence of m1FA in the complex increased only in the presence of Pi, while the weak fluorescence of FB appeared unaffected, independently of Pi. Anal. of the emission, excitation and absorption spectra of enzyme-ligand mixts. pointed to fluorescence resonance energy transfer (FRET) from protein tyrosine residue(s) to FA and m6FA base moieties, as a major mechanism of protein fluorescence quenching. With the non-inhibitor M2FA, fluorescence emission and excitation spectra were purely additive. Effects of enzyme-FA, or enzyme-m6FA, interactions on nucleoside excitation and emission spectra revealed shifts in tautomeric equil. of the bound ligands. With FA, which exists predominantly as the N(1)-H tautomer in soln., the proton N(1)-H is shifted to N(2), independently of the presence of Pi. Complex formation with m6FA in the absence of Pi led to a shift of the amino-imino equil. in favor of the imino species, and increased fluorescence at 350 nm; by contrast, in the presence of Pi, the equil. was shifted in favor of the amino species, accompanied by higher fluorescence at 430 nm, and a higher affinity for the enzyme, with a

dissocn. const. Kd=0.5.+-.0.1 .mu.M, two orders of magnitude lower than that for m6FA in the absence of Pi (Kd=46.+-.5 .mu.M). The latter was confirmed by anal. of quenching of enzyme fluorescence according to a modified Stern-Volmer model. Fractional accessibility values (fa) varied from 0.31 for m1FA to 0.70 for FA, with neg. cooperative binding of m1FA and FB, and non-cooperative binding of FA and m6FA. For all nucleoside ligands, the best model describing binding stoichiometry was one ligand per native enzyme hexamer. Fluorescence decays of PNP, FA and their mixts. were best fitted to a sum of two exponential terms, with av. lifetimes (.ltbbrac..tau..rtbbrac.) affected by their interactions. Complex formation resulted in a 2-fold increase in .ltbbrac..tau..rtbbrac. of FA, and a 2-fold decrease in .ltbbrac..tau..rtbbrac. of enzyme fluorescence. The amplitude of the long-lifetime component also increased, confirming the shift of the tautomeric equil. in favor of the N(2)-H species. The findings have been examd. in relation to enzyme-nucleoside binding deduced from structural studies.

CC 7-3 (Enzymes)

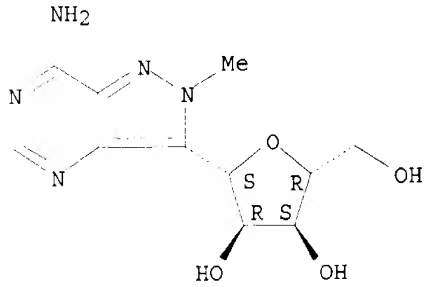
IT 6742-12-7, Formycin A 9030-21-1, Purine nucleoside phosphorylase
13877-76-4, Formycin B **42204-46-6** 51222-28-7 70421-28-2
70421-29-3
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(induced tautomeric shifts and enzyme ligand fluorescence resonance energy transfer upon binding of formycin A to purine nucleoside phosphorylase)

IT **42204-46-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(induced tautomeric shifts and enzyme ligand fluorescence resonance energy transfer upon binding of formycin A to purine nucleoside phosphorylase)

RN 42204-46-6 HCAPLUS

CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 27 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:443336 HCAPLUS

DOCUMENT NUMBER: 117:43336

TITLE: Formycins A and B and some analogs: selective inhibitors of bacterial (Escherichia coli) purine nucleoside phosphorylase

AUTHOR(S): Bzowska, Agnieszka; Kulikowska, Ewa; Shugar, David

CORPORATE SOURCE: Inst. Exp. Phys., Univ. Warsaw, Warsaw, Pol.
SOURCE: Biochim. Biophys. Acta (1992), 1120(3), 239-47
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Formycin B (FB), a moderate inhibitor (Ki .apprx. 100 .mu.M) of mammalian purine nucleoside phosphorylase (PNP), and formycin A (FA), which is totally inactive vs. the mammalian enzyme, are both effective inhibitors of the bacterial (E. coli) enzyme (Ki .apprx. 5 .mu.M). Examn. of a series of N-Me analogs of FA and FB led to the finding that N(6)-methyl-FA, virtually inactive vs. the mammalian enzyme, is the most potent inhibitor of E. coli purine nucleoside phosphorylase (Ki .apprx. 0.3 .mu.M) at neutral pH. Inhibition is competitive not only with respect to inosine, but also relative to 7-Me guanosine and 7-methyladenosine, as substrates. Both oxoformycins A and B are relatively poor inhibitors. For the most potent inhibitor, N(6)-methyl-FA, it was shown that the enzyme preferentially binds the neutral, and not the cationic, form. In accordance with this the neutral,but not the cationic form, of the structurally related N(1)-methyladenosine was an excellent substrate. Reported data on tautomerism of formycins were profited from, and extended, to infer which tautomeric species and ionic forms are the active inhibitors. A commercially available (Sigma) bacterial PNP, of unknown origin, was shown to differ from the E. coli enzyme by its inability to phosphorylzeadenosine; this enzyme was also resistant to FA and FB. These findings have been extended to provide a detailed comparison of the substrate/inhibitor properties of PNP from various microorganisms.

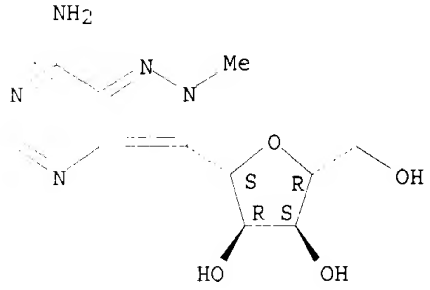
CC 7-3 (Enzymes)
Section cross-reference(s): 1, 10, 15

IT 6742-12-7, Formycin A 13877-76-4, Formycin B 19246-88-9, Oxoformycin B **42204-46-6** 51222-28-7 70421-28-2 74024-59-2 94856-89-0, Oxoformycin A
PL: BIOL (Biological study)
(purine nucleoside phosphorylase of Escherichia coli inhibition by, structure in relation to)

IT **42204-46-6**
PL: BIOL (Biological study)
(purine nucleoside phosphorylase of Escherichia coli inhibition by, structure in relation to)

RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 3 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:172780 HCAPLUS

DOCUMENT NUMBER: 106:172780
TITLE: Biological action of pyrazolopyrimidine derivatives against Trypanosoma cruzi. Studies in vitro and in vivo
AUTHOR(S): Avila, Jose Luis; Polegre, Maria Argelia; Robins, Roland K.
CORPORATE SOURCE: Inst. Biomed., Caracas, 1010A, Venez.
SOURCE: Comp. Biochem. Physiol., C: Comp. Pharmacol. Toxicol. (1987), 86C(1), 49-54
CODEN: CBPCEE; ISSN: 0742-8413
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The capacity of 54 different pyrazolo(3,4-d) or (4,3-d)pyrimidine derivs. to inhibit T. cruzi epimastigote and trypomastigote multiplication, and for some of them their chemotherapeutic activity, was evaluated. Six pyrazolo(3,4-d)pyrimidines showed inhibitory activity against epimastigote forms, 4-aminopyrazolo(3,4-d)pyrimidine being the most active, 5-fold more so than 4-hydroxypyrazolo(3,4-d)pyrimidine. Neither compd. was active against freshly isolated trypomastigotes, suggesting biochem. differences between culture and bloodstream forms of T. cruzi. On both epimastigote and trypomastigote forms, 7-amino-3-.beta.-D-ribofuranosylpyrazolo(4,3-d)pyrimidine (FoA) was .apprx.2-fold more active than 7-hydroxy-3-.beta.-D-ribofuranosylpyrazolo(4,3-d)pyrimidine (FoB); however, when tested on T. cruzi-infected mice, only FoB exhibited significant chemotherapeutic activity. Previous results suggest that, except for FoB and FoA, pyrazolopyrimidine insensitivity is trypomastigote-specific and drug insensitivity is lost when trypomastigotes transform into epimastigotes and vice versa.

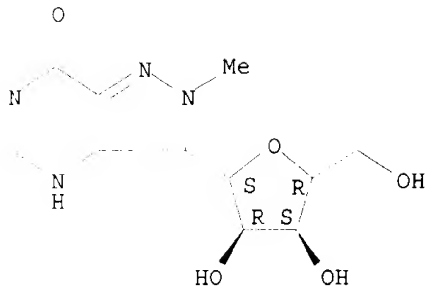
CC 10-5 (Microbial Biochemistry)
Section cross-reference(s): 1

IT 73-24-5, biological studies 271-80-7 315-30-0 938-55-6 3258-05-7
5334-64-5 5401-48-9 5405-64-1 5413-96-7 5441-46-3 5444-29-1
5444-73-5 5472-41-3 6014-06-8 6284-74-8 6742-12-7 13263-91-7
13351-68-3 13877-76-4 16220-07-8 17318-21-7 39102-66-4
51088-28-9 **51481-59-5** 56477-17-9 58360-86-4 74024-59-2
80206-18-4 83255-86-1 85426-75-1 90085-12-4 90914-31-1
90914-34-4 90914-42-4 91492-85-2 99867-27-3 99973-41-8
100124-91-2 101744-61-0 102353-66-2 102353-67-3 102353-68-4
102353-69-5 102353-70-8 102353-71-9 102353-72-0 102353-73-1
102353-74-2 102353-75-3 102353-76-4 102353-77-5 102353-78-6
102353-79-7 102353-80-0
RL: BIOL (Biological study)
(trypanosomicidal activity of)

IT **51481-59-5**
RL: BIOL (Biological study)
(trypanosomicidal activity of)

RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 4 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:454102 HCAPLUS
DOCUMENT NUMBER: 105:54102
TITLE: Action of pyrazolopyrimidine derivatives on Trypanosoma rangeli culture forms
AUTHOR(S): Avila, Jose Luis; Polegre, Maria A.; Robins, Roland K.
CORPORATE SOURCE: Inst. Biomed., Carcas, 1010A, Venez.
SOURCE: Comp. Biochem. Physiol., C: Comp. Pharmacol. Toxicol.. (1986), 83C(2), 291-4
CODEN: CBPCEE; ISSN: 0742-8413
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The capacity of 54 different pyrazolo(3,4-d)pyrimidines [e.g. I; R1 = H, Cl, OH, MeS, benzylamino; R2 = H, (un)substituted amino; R3 = H, Me, p-bromophenyl, .beta.-D-ribofuranosyl, etc.] of pyrazolo(4,3-d)pyrimidines [e.g. II; R1 = OH, Me, NH2, selenoxo, etc.; R2 = H or Me] to inhibit the multiplication of T. rangeli culture forms was evaluated. Among I, 14 derivs. showed trypanostatic activity, 4-aminopyrazolo(3,4-d)pyrimidine (APP) [2380-63-4] being the most active, with 4-hydroxypyrazolo(3,4-d)pyrimidine [315-30-0] lacking trypanostatic activity. 7-Hydroxy-3-.beta.-D-ribofuranosylpyrazolo(4,3-d)pyrimidine [6742-12-7] was as active as 7-amino-3-.beta.-D-ribofuranosylpyrazolo(4,3-d)pyrimidine [13877-76-4], both compds. being 5-fold less inhibitory than APP. The chem. analogy to hypoxanthine or inosine of pyrazolo(3,4-d)- and pyrazolo(4,3-d)pyrimidine, resp., is not absolutely crit. for antihyponosomal activity, as different modifications on the heterocyclic ring did not abolish the inhibitory activity of these compds.

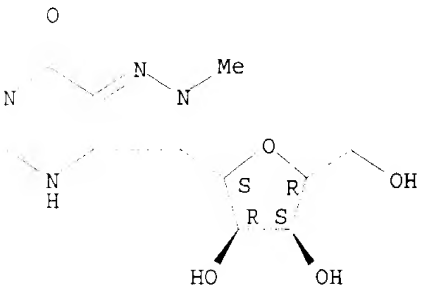
CC 1-3 (Pharmacology)

IT 271-80-7 315-30-0 2380-63-4 3258-05-7 5334-64-5 5401-48-9
5405-64-1 5413-96-7 5441-46-3 5444-29-1 5444-73-5 5472-41-3
6014-06-8 6284-74-8 6742-12-7 13264-01-2D, derivs. 13351-68-3
13877-76-4 16220-07-8 17318-21-7 23002-57-5 39102-66-4
51088-28-9 **51481-59-5** 56477-17-9 58360-86-4 74024-59-2
80206-18-4 83255-86-1 85426-75-1 90085-12-4 90914-31-1
90914-34-4 90914-42-4 91492-85-2 99867-27-3 99973-41-8
100124-91-2 101744-61-0 102353-66-2 102353-67-3 102353-68-4
102353-69-5 102353-70-8 102353-71-9 102353-72-0 102353-73-1
102353-74-2 102353-75-3 102353-76-4 102353-77-5 102353-78-6
102353-79-7 102353-80-0 102353-81-1
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(antitrypanosomal activity of, structure in relation to)

IT **51481-59-5**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(antitrypanosomal activity of, structure in relation to)
RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:454101 HCAPLUS
DOCUMENT NUMBER: 105:54101
TITLE: Action of pyrazolopyrimidine derivatives on american Leishmania species promastigotes
AUTHOR(S): Avila, Jose Luis; Polegre, Maria A.; Avila, Angela; Robins, Roland K.
CORPORATE SOURCE: Inst. Biomed., Caracas, 1010A, Venez.
SOURCE: Comp. Biochem. Physiol., C: Comp. Pharmacol. Toxicol., (1986), 83C(2), 285-9
CODEN: CBPCEE; ISSN: 0742-8413
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The capacity of 54 different pyrazolo[(3,4-d)pyrimidines [e.g. I; R1 = H, Cl, OH, MeS, benzylamino; R1 = H, (un)substituted amino; R3 = H, Me, p-bromophenyl, .beta.-D-ribofuranosyl, etc.] or pyrazolo-(4,3-d)-pyrimidines [e.g. II; R1 = OH, Me, NH2, selenoxo, etc.; R2 = H or Me] to inhibit American Leischmania promastigote multiplication was evaluated. Among I, 8 derivs. showed leishmanistatic activity, 4-aminopyrazolo(3,4-d)-pyrimidine (APP) [2380-63-4] being the most active, about 8-fold more than 4-hydroxypyrazolo-(3,4-d)-pyrimidine [315-30-0]. 7 Hydroxy-3-.beta.-D-ribofuranosylpyrazolo-(4,3-d)-pyrimidine [6742-12-7] was as active as 7-amino-3-.beta.-D-ribofuranosylpyrazolo-(4,3-d)-pyrimidine [13877-76-4], a situation different to that found for pyrazolo-(3,4-d)-pyrimidines. Furthermore, different chem. modifications in formycin structure did not modify inhibitory effects. The chem. analogy to hypoxanthine or inosine of pyrazolo-(3,4-d)- and pyrazolo-(4,3-d)-pyrimidine, resp., is not absolutely crit. for antileishmanial activity, as different modifications on the heterocyclic ring did not abolish the inhibitory activity of these compds.
CC 1-3 (Pharmacology)
IT 271-80-7 315-30-0 2380-63-4 3258-05-7 5334-64-5 5401-48-9
5405-64-1 5413-96-7 5441-46-3 5444-29-1 5444-73-5 5472-41-3
6014-06-8 6284-74-8 6742-12-7 13264-01-2D, derivs. 13351-68-3
13877-76-4 16220-07-8 17318-21-7 23002-57-5 39102-66-4
51088-28-9 **51481-59-5** 56477-17-9 58360-86-4 74024-59-2
80206-18-4 83255-86-1 85426-75-1 90085-12-4 90914-31-1
90914-34-4 90914-42-4 91492-85-2 99867-27-3 99973-41-8
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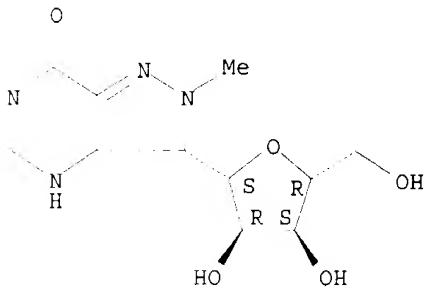
102353-69-5 102353-70-8 102353-71-9 102353-72-0 102353-73-1
102353-74-2 102353-75-3 102353-76-4 102353-77-5 102353-78-6
102353-79-7 102353-80-0 102353-81-1
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(antileishmanial activity of, structure in relation to)

IT **51481-59-5**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(antileishmanial activity of, structure in relation to)

RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:589207 HCAPLUS
DOCUMENT NUMBER: 103:189207
TITLE: Inosine analogs as anti-leishmanial agents
AUTHOR(S): Rainey, Petrie; Nolan, Patricia A.; Townsend, Leroy B.; Robins, Roland K.; Fox, Jack J.; Secrist, John A., III; Santi, Daniel V.
CORPORATE SOURCE: Sch. Med., Univ. California, San Francisco, CA, 94143, USA
SOURCE: Pharm. Res. (1985), (5), 217-20
CODEN: PHREEB
DOCUMENT TYPE: Journal
LANGUAGE: English

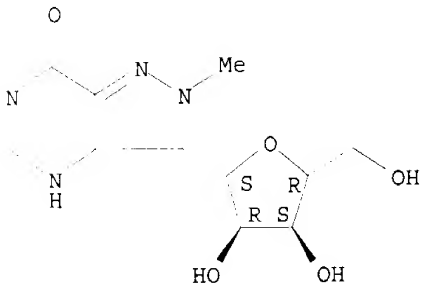
AB Several criteria were used to select a no. of inosine analogs as potential growth inhibitors of the protozoan parasite Leishmania tropica. Of 9 compds. tested, 7 showed a high degree of selective toxicity towards L. tropica promastigotes as compared to mouse L1210 cells; these include analogs of formycin B [13877-76-4], 7-substituted analogs of 7-deazainosine, and analogs of inosine in which the sugar moiety has been modified to confer metabolic stability. The metab. of 7-deazainosine in L. tropica promastigotes was shown to involve conversion to cytotoxic adenosine nucleotide analogs (tubercidin derivs.) that become incorporated into RNA. The results suggest several new classes of compds. which have potential as anti-leishmanial agents. Structure-activity relations are discussed.

CC 1-3 (Pharmacology)

IT 58-63-9D, analogs 2862-16-0 13263-91-7 13877-76-4 16975-94-3
22242-94-0 22242-96-2 24386-96-7 39102-63-1 **51481-59-5**
74024-59-2 98983-40-5
RL: BAC (Biological activity or effector, except adverse); BIOL

(Biological study)
(antileishmanial activity of, structure in relation to)
IT **51481-59-5**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(antileishmanial activity of, structure in relation to)
RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

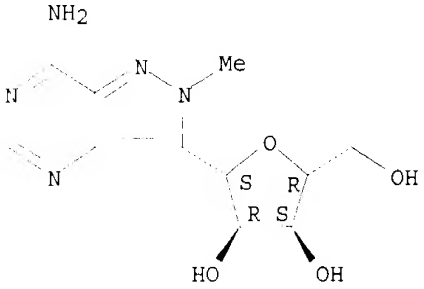
Absolute stereochemistry.



L5 ANSWER 7 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:185417 HCAPLUS
DOCUMENT NUMBER: 102:185417
TITLE: Synthesis of 1-methyl-3-.beta.-D-ribofuranosylpyrazolo[4,3-d]-pyrimidin-7(6H)-selone and certain related nucleosides and nucleotides
AUTHOR(S): Ugarkar, Bheemarao G.; Robins, Roland K.; Revankar, Ganapathi R.
CORPORATE SOURCE: Cancer Res. Cent., Brigham Young Univ., Provo, UT, 84602, USA
SOURCE: Nucleosides Nucleotides (1984), 3(3), 233-44
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1-Methylformycin B (I; Z = O) and its S and Se analogs (I; Z = S, Se) were prepd. from 1-methylformycin (II; R = H). Deamination of II (R = H) with liq. NOCl in DMF gave almost quant. I (Z = O), which was then converted into I (Z = S, Se). II (R = H) was also phosphorylated to give II [R = (HO)2P(O), (III)]. I (Z = Se) and III were potent inhibitors of growth of L1210 and P388 leukemia.
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT **42204-46-6**
RL: RCT (Reactant)
(deamination of)
IT 96221-16-8P **96221-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and neutralization of)
IT **51481-59-5P** 96221-21-5P 96221-24-8P 96221-25-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **42204-46-6**
RL: RCT (Reactant)
(deamination of)

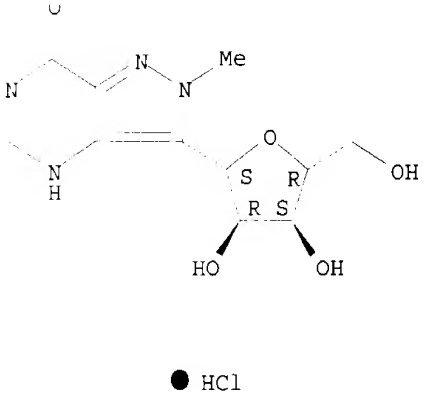
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



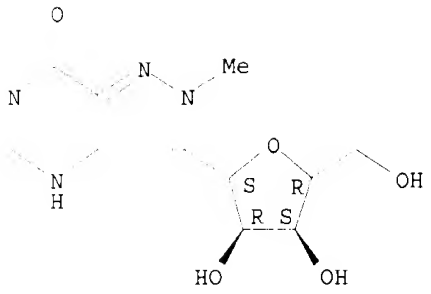
IT **96221-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and neutralization of)
RN 96221-17-9 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **51481-59-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 8 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:167081 HCAPLUS
DOCUMENT NUMBER: 102:167081
TITLE: A simple oxidation of formycin to oxoformycin and oxoformycin B. Synthesis of 6-methyloxoformycin, a C-nucleoside analog of doridosine
AUTHOR(S): Ugarkar, Bheemarao G.; Revankar, Ganapathi R.; Robins, Roland K.
CORPORATE SOURCE: Cancer Res. Cent., Brigham Young Univ., Provo, UT, 84602, USA
SOURCE: J. Heterocycl. Chem. (1984), 21(6), 1865-70
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A simple, high-yield procedure was developed for the direct oxidn. of formycin (I) to oxoformycin (II) and oxoformycin B (III). Treatment of I with Br/H2O gave II. A similar treatment of formycin B gave III. Upon prolonged exposure of either I or II to Br/H2O at reflux temp., conversion to III occurred in good yield. Application of this procedure to 1-methylformycin, 1-methylformycin B and 2-methylformycin gave 1-methyloxoformycin, 1-methyloxoformycin B and 2-methyloxoformycin, resp. This selective oxidn. of 6-methylformycin gave 7-amino-6-methyl-3-.beta.-D-ribofuranosylpyrazolo[4,3-d]pyrimidin-5(4H)-one, a C-nucleoside analog of doridosine. A similar oxidn. of 1,6-dimethylformycin B gave 1,6-dimethyloxoformycin B. This direct introduction of the 5-oxo function into the pyrazolo[4,3-d]pyrimidine ring appears to be due to the attack of Br+ at N-4, followed by the addn. of water to C-5 and subsequent elimination of HBr.

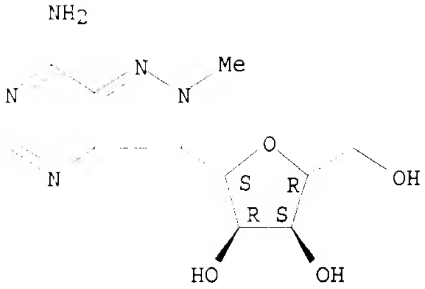
CC 33-9 (Carbohydrates)

IT **42204-46-6 51481-59-5** 70421-29-3 74024-57-0
RL: RCT (Reactant)
(oxidn. of, with bromine-water)

IT **42204-46-6 51481-59-5**
RL: RCT (Reactant)
(oxidn. of, with bromine-water)

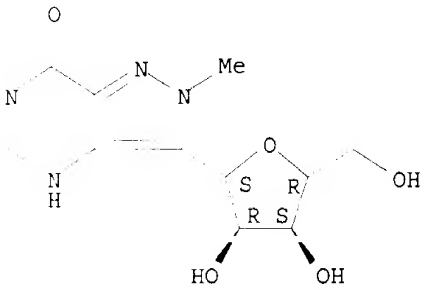
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



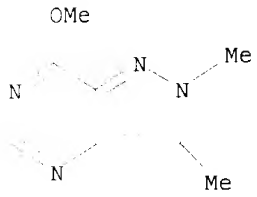
RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 9 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:472691 HCAPLUS
DOCUMENT NUMBER: 101:72691
TITLE: Acyclo analogs of formycin A
AUTHOR(S): Griengl, H.; Guenzl, F.
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Graz, Graz, A-8010, Austria
SOURCE: J. Heterocycl. Chem. (1984), 21(2), 505-8
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Pyrazolopyrimidine I (R = Cl, R1 = H, R2 = Me) treated, with MeOH-HCl, followed by methylation and bromination, gave I (R = OMe, R1 = Me, R2 = CH2Br, II). Treatment of II with HOCH2CH2OH gave I (R2 = CH2OCH2CH2OH, III), which was aminated to give I (R = NH2, R1 = Me, R2 = CH2OCH2CH2OH, IV), an acyclic analog of formycin A. III and IV were inactive in the L 1210 leukemia cell cloning assay and several antiviral assays.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 33
IT 22283-32-5P **91225-97-7P** 91225-99-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **91225-97-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 91225-97-7 HCAPLUS

CN 2H-Pyrazolo[4,3-d]pyrimidine, 7-methoxy-2,3-dimethyl- (9CI) (CA INDEX NAME)

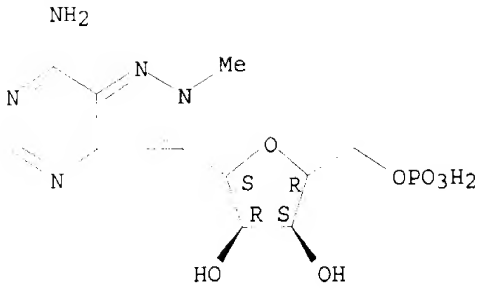


L5 ANSWER 10 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:450520 HCAPLUS
DOCUMENT NUMBER: 101:50520
TITLE: Continuous fluorimetric assay of 5'-nucleotidase with formycin 5'-phosphate as substrate, and its application to properties of substrates and inhibitors
AUTHOR(S): Wierzchowski, Jacek; Lassota, Piotr; Shugar, David
CORPORATE SOURCE: Inst. Phys., Acad. Agric., Poznan, 60-637, Pol.
SOURCE: Biochim. Biophys. Acta (1984), 786(3), 170-8
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The modifications in UV absorption and fluorescence emission accompanying dephosphorylation of formycin 5'-phosphate may be employed for the continuous assay of 5'-nucleotidase (EC 3.1.3.5) activity. The sensitivity of the fluorometric method is addnl. enhanced by coupling the reaction with adenosine deaminase, which deaminates formycin more rapidly than adenosine. The final product is then formycin B, which is nonfluorescent at neutral pH and only slightly so at alk. pH. The fluorescence procedure permits the use of substrate concns. as low as 1 .mu.M in a 10 mm cuvette. Details are described for the use of the foregoing systems to follow continuously the kinetics as well as the properties of a no. of substrate and inhibitor analogs of the enzyme from snake venom. Kinetic parameters are presented and compared with reported values for the enzyme from other sources. In particular, the pH dependence of the inhibitory properties of nucleoside 5'-diphosphates (NDP) points to the non-dissocd. form, NDP2-, as the potent inhibitory species. An esp. useful inhibitor is adenosine .alpha.,.beta.-methylene-5'-pyrophosphate, because of its higher pK value for the .beta.-phosphate secondary hydroxyl ionization, so that it is the most suitable inhibitor for kinetic and in vivo investigations over a broad pH range. The spectral properties of formycin analogs are tabulated, and ref. made to their potential applications to other enzyme systems.

CC 7-1 (Enzymes)
IT 61-19-8, reactions **91034-38-7**
RL: RCT (Reactant)
(reaction of, with 5'-nucleotidase, kinetics of)
IT **91034-38-7**
RL: RCT (Reactant)
(reaction of, with 5'-nucleotidase, kinetics of)
RN 91034-38-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 5-(dihydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

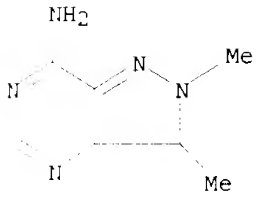
Absolute stereochemistry.



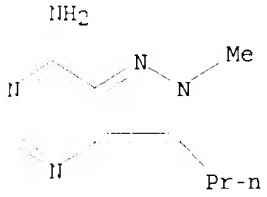
L5 ANSWER 11 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:139399 HCAPLUS
DOCUMENT NUMBER: 98:139399
TITLE: Sensitive fluorimetric assay for adenosine deaminase with formycin as substrate; and substrate and inhibitor properties of some pyrazolopyrimidine and related analogs
AUTHOR(S): Wierzchowski, Jacek; Shugar, David
CORPORATE SOURCE: Dep. Phys., Acad. Agric., Poznan, 60-637, Pol.
SOURCE: Z. Naturforsch., C: Biosci. (1983), 38C(1-2), 67-73
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The nucleoside antibiotic, formycin (I), a structural analog of adenosine (II), is deaminated approx. 10-fold faster by adenosine deaminase (III) than II itself, and is therefore a superior substrate for both routine assays and kinetic studies with purified III. The luminescence properties of I were used to develop a fluorometric assay for III which was considerably more sensitive than the spectrophotometric procedure widely employed with II as substrate. Examples are presented of its application to routine assays of III levels in cellular exts., as well as to kinetic studies with purified III, including the properties of some pyrazolopyrimidine and purine substrates and inhibitors.

CC 7-1 (Enzymes)
IT 700-00-5 1818-71-9 2380-63-4 2715-68-6 3373-53-3 5334-99-6
51222-25-4 57573-29-2 76424-52-7 76424-70-9
76424-71-0 85179-59-5
RL: BIOL (Biological study)
(adenosine deaminase inhibition by, kinetics of)
IT 58-61-7, reactions 73-24-5, reactions 3258-05-7 13351-68-3
42204-46-6 76424-61-8
RL: RCT (Reactant)
(reaction of, with adenosine deaminase, kinetics of)
IT **51222-25-4 76424-71-0**
RL: BIOL (Biological study)
(adenosine deaminase inhibition by, kinetics of)
RN 51222-25-4 HCAPLUS
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2,3-dimethyl- (9CI) (CA INDEX NAME)

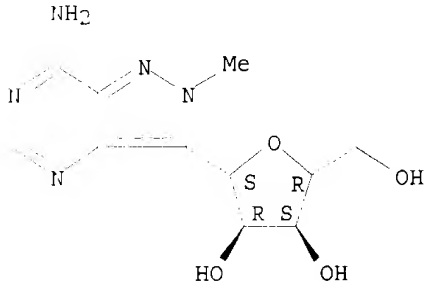


RN 76424-71-0 HCAPLUS
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2-methyl-3-propyl- (9CI) (CA INDEX NAME)



IT **42204-46-6**
PL: RCT (Reactant)
(reaction of, with adenosine deaminase, kinetics of)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 12 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:472675 HCAPLUS
DOCUMENT NUMBER: 97:72675
TITLE: Luminescence studies on formycin, its aglycone, and their N-methyl derivatives: tautomerism, sites of protonation, and phototautomerism
AUTHOR(S): Wierzchowski, Jacek; Shugar, David
CORPORATE SOURCE: Dep. Biophys., Univ. Warsaw, Warsaw, 02-089, Pol.
SOURCE: Photochem. Photobiol. (1982), 35(4), 445-58
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The luminescence spectra of formycin A (I), its aglycone, and various N-Me

derivs., at room temp. and at 77 K indicated that they consist of 2 tautomeric species, N(1)H and N(2)H, both of which emit at 300 and 77 K; they could be distinguished by the location of the emission max., esp. for phosphorescence and quantum yields for emission. The emission spectra of the protonated forms of the aglycone and its N-Me derivs. indicated that fluorescence of the cations originated from the forms protonated on N(4), with forms protonated on N(6) contributing to the phosphorescence at 77K. The major tautomeric form of the formycin cation is N(1)H,N(4)H+, with some contribution by N(2)H,N(4)H+. Photodissocn. of a proton from the pyrazole ring of the formycin cation occurred in acid medium at room temp., leading to formation in the state S1 of the tautomeric species N(4)H. The proposed mechanism of phototautomerization is supported by a study of solvent and salt effects.

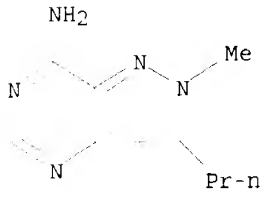
CC 33-3 (Carbohydrates)
Section cross-reference(s): 22, 26, 28

IT 82538-37-2 82538-38-3 82538-39-4 82538-40-7 82538-41-8
82538-42-9 **82538-43-0 82538-44-1** 82538-45-2
82538-46-3 82538-47-4
RL: RCT (Reactant)
(luminescence studies on, (photo)tautomerism in relation to)

IT 6742-12-7 **42204-46-6** 51222-28-7 70421-28-2 70421-29-3
76424-61-8 76424-70-9 **76424-71-0** 76424-72-1 76424-73-2
76424-75-4 76424-77-6
RL: RCT (Reactant)
(luminescence studies on, protonation and (photo)tautomerism in relation to)

IT **82538-43-0 82538-44-1**
RL: RCT (Reactant)
(luminescence studies on, (photo)tautomerism in relation to)

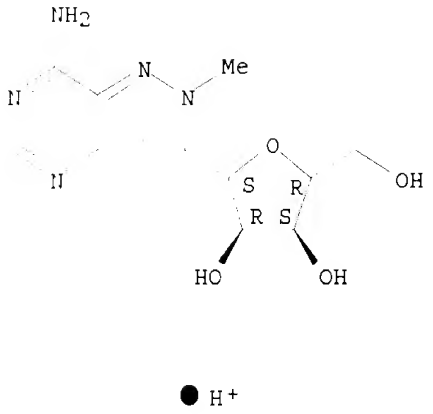
RN 82538-43-0 HCAPLUS
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2-methyl-3-propyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H+

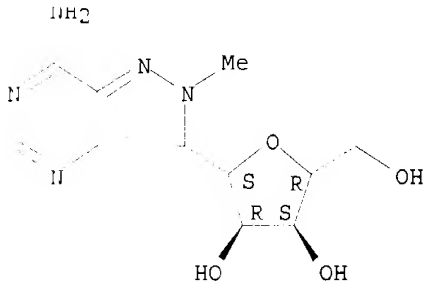
RN 82538-44-1 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, conjugate monoacid, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

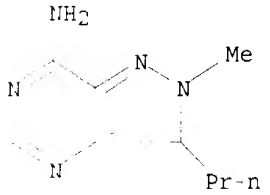


IT **42204-46-6 76424-71-0**
RL: RCT (Reactant)
(luminescence studies on, protonation and (photo)tautomerism in relation to)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 76424-71-0 HCAPLUS
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2-methyl-3-propyl- (9CI) (CA INDEX NAME)



L5 ANSWER 13 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:65608 HCAPLUS
DOCUMENT NUMBER: 94:65608
TITLE: Analogs of formycins A and B: synthesis and some

properties of methyl derivatives of 7-amino and 7-keto pyrazolo[4,3-d]pyrimidines

AUTHOR(S): Wierzchowski, Jacek; Kusmierek, Jaroslaw; Giziewicz, Jerzy; Salvi, D.; Shugar, David

CORPORATE SOURCE: Dep. Biophys. Inst. Exp. Phys., Univ. Warsaw, Warsaw, 02-089, Pol.

SOURCE: Acta Biochim. Pol. (1980), 27(1), 35-56
CODEN: ABPLAF; ISSN: 0001-527X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Cyclocondensation of aminopyrazoles I (R = H, Et), obtained by sequential nitration, esterification, and hydrogenation of pyrazolecarboxylic acid II, with formamide gave pyrazolopyrimidines III (X = O, R = H, Et). Sulfuration of the latter compds. with P2S5 gave III (X = S, R = H, Et), amination of which with HNR1R2 (R1, R2 = H, Me) gave IV. Me and di-Me derivs. of IV were then prepd. by treating IV with CH2N2 in MeOH, and Me iodide in DMF. All 4 possible ring mono-methyl derivs. of IV (R = R1 = R2 = H) (V) were prepd. by use of different methylating agents. UV and NMR spectra and pKa values for the methyl derivs. of V showed that the N6-Me deriv. of V exists in the imino form in contrast to the amino form in the N1-Me deriv. of adenine, but similar to the imino form of the N1-Me derivs. of C-9 substituted adenines.

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

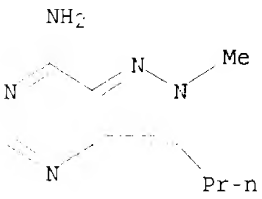
IT 76424-57-2P 76424-58-3P 76424-61-8P 76424-70-9P **76424-71-0P**
PL: PCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methylation of)

IT 76424-54-9P 76424-59-4P 76424-63-0P 76424-64-1P 76424-66-3P
76424-67-4P 76424-68-5P 76424-69-6P 76424-72-1P 76424-74-3P
76424-76-5P 76424-78-7P 76424-79-8P **76424-80-1P**
76424-82-3P 76434-34-9P
PL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **76424-71-0P**
PL: PCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methylation of)

RN 76424-71-0 HCAPLUS

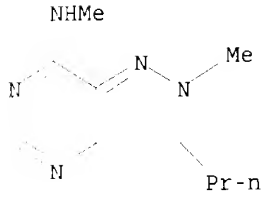
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2-methyl-3-propyl- (9CI) (CA INDEX NAME)



IT **76424-80-1P**
PL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 76424-80-1 HCAPLUS

CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, N,2-dimethyl-3-propyl- (9CI) (CA INDEX NAME)

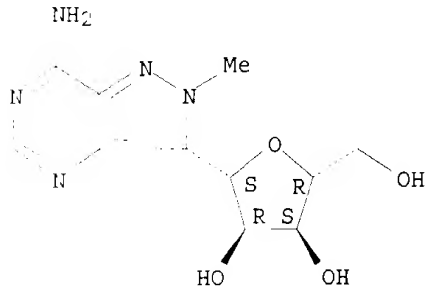


L5 ANSWER 14 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:426714 HCAPLUS
DOCUMENT NUMBER: 93:26714
TITLE: Pyrazolo[4,3-d]pyrimidine nucleosides. 9. Studies on the isomeric N-methylformycins
AUTHOR(S): Lewis, Arthur F.; Townsend, Leroy B.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109, USA
SOURCE: J. Am. Chem. Soc. (1980), 102(8), 2817-22
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 4-Methylformycin (I) and 6-methylformycin (II) were prepd. by methylation of formycin with MeI in DMF. Structural assignments of I and II were based on UV, 1H NMR, and 13C NMR data. N-7-Methylformycin (III) was resynthesized by an alternate route and comparisons of the physicochem. Properties of all five of the mono-N-methylformycins are presented. II was unstable in aq. soln. yielding 3 products, formycin B, III and 6-methylformycin B. 6-Methylformycin B, 4-methylformycin B, and 1-methylformycin B were prepd. by a reaction of NOCl with II, I, and 1-methylformcyin, resp. 1-Methyl-, 2-methylformycin, and III showed significant cytotoxicity to L-1210 cells in culture.

CC 33-7 (Carbohydrates)
Section cross-reference(s): 1, 28
IT **42204-46-6**
RL: PRP (Properties)
(spectra of)
IT **42204-46-6**
RL: PRP (Properties)
(spectra of)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 15 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:193903 HCAPLUS
DOCUMENT NUMBER: 92:193903
TITLE: Nucleoside 5'-phosphates. Enzymic phosphorylation of nucleosides to the 5'-phosphates
AUTHOR(S): Gizliewicz, Jerzy; Shugar, David
CORPORATE SOURCE: Inst. Biochem. Biophys., Acad. Sci., Warsaw, 02-532, Pol.
SOURCE: Nucl. Acid Chem. (1978), Volume 2, 955-61. Editor(s): Townsend, Leroy B.; Tipson, R. Stuart. Wiley: New York, N. Y.
CODEN: 42TBAU
DOCUMENT TYPE: Conference
LANGUAGE: English

AB Wheat shoot phosphotransferase was used for the phosphorylation of nucleosides and the products were fractioned on Dowex-1 (HCO3- or HCO2-) ion exchange resin. Thus, nucleoside (0.06M) and p-nitrophenyl phosphate (0.6M) were dissolved in H2O and pH brought to 4 by HOAc addn. An equal vol. of the enzyme prepn. was added and the mixt. was incubated 18-24 h at 37.degree.. The reaction was terminated by a brief boil and the cooled mixt. was extd. with Et2O to remove the released p-nitrophenol. The aq. soln., freed of Et2O was dild., made alk. (pH .apprx.8), and loaded onto the column. Readily protonated nucleosides that are reasonably stable in acid medium were sepd. on the HCO2- form of the resin. After washing with H2O to remove the unreacted nucleoside the nucleotide was eluted with a gradient of HCO2H 0-1M. The fraction of phosphorylation products including formycin 5'-phosphate is shown.

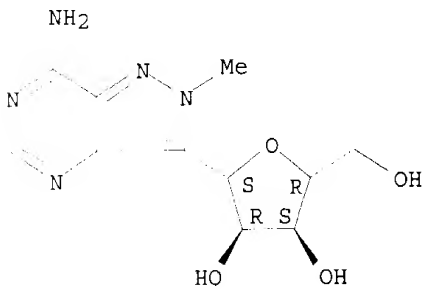
CC 9-6 (Biochemical Methods)
Section cross-reference(s): 7

IT 50-91-9 65-46-3 1445-07-4 2140-72-9 4546-54-7 5746-29-2
16710-13-7 20594-00-7 33000-97-4 34218-86-5 **42204-46-6**
50356-36-0 50499-40-6 51222-28-7
RL: ANST (Analytical study)
(phosphorylation of, by phosphotransferase of wheat)

IT **42204-46-6**
RL: ANST (Analytical study)
(phosphorylation of, by phosphotransferase of wheat)

RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 16 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:209 HCAPLUS

DOCUMENT NUMBER: 92:209
TITLE: N-methylformycins. Reactivity with adenosine deaminase, incorporation into intracellular nucleotides of human erythrocytes and L1210 cells and cytotoxicity to L1210 cells
AUTHOR(S): Crabtree, Gerald W.; Agarwal, Ram P.; Parks, Robert E., Jr.; Lewis, Arthur F.; Wotring, Linda L.; Townsend, Leroy B.
CORPORATE SOURCE: Div. Biol. Med., Brown Univ., Providence, RI, USA
SOURCE: Biochem. Pharmacol. (1979), 28(9), 1491-500
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1-Methylformycin [51222-28-7], which readily assumed the anti conformation, showed no substrate activity for erythrocyte adenosine deaminase (I) [9026-93-1], whereas 2-methylformycin [**42204-46-6**], which was presumably fixed in the syn position, showed substrate activity for I .apprx.4 times greater than that of adenosine; N7-methylformycin [13351-68-3] also showed substrate activity for I. Thus, conformation was not important in detg. the substrate activity to I of an adenosine analog but the 7 position (purine ring structure) was important for the binding of adenosine and its analogs to the active site of I. Formycin (II) and its 1-Me, 2-Me, and 7-Me derivs. had similar toxicity to L1210 cells, whereas formycin B [13877-76-4] and other N-Me derivs. were inactive. The compds. that showed pronounced cytotoxicity to L1210 cells were also capable of forming nucleotides in human erythrocytes or L1210 cells if deamination was prevented either by the mol. structure of the analog or by a I inhibitor. The potential use of the N-Me II derivs. (alone or combined with a I inhibitor) as cytotoxic or antiviral agents is discussed.

CC 1-3 (Pharmacodynamics)

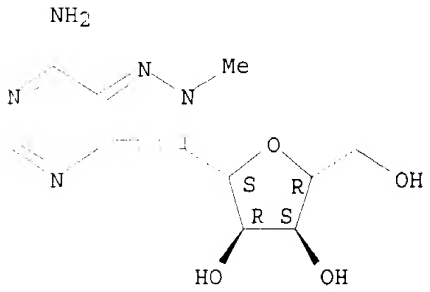
IT 13351-68-3 13877-76-4 **42204-46-6** 51222-28-7 70421-28-2 70421-29-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(adenosine deaminase reactivity and cytotoxicity of)

IT **42204-46-6**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(adenosine deaminase reactivity and cytotoxicity of)

RN 42204-46-6 HCAPLUS

CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



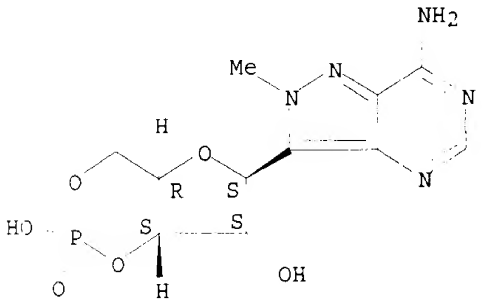
L5 ANSWER 17 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:611773 HCAPLUS

DOCUMENT NUMBER: 91:211773
TITLE: Formycin 3',5'-cyclic phosphate
INVENTOR(S): Umezawa, Sumio; Umezawa, Hamao; Kawamura, Kenji; Makabe, Osamu
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54088295	A2	19790713	JP 1977-154396	19771223
JP 61002072	B4	19860122		

AB A mixt. of 4.5 mL (MeO)3PO, 0.6 mL POCl3, and 1 g formcyin was stirred 2 h at -5.degree. and treated with Dowex 50W .times. 8 (H+) to give 845 mg formycin-5'-phosphate (I). Dicyclohexylcarbodiimide (1.65 g) in pyridine was added to a refluxing mixt. of 1.46 g I and 200 mL (Me2N)3PO in pyridine over 1 h, the whole refluxed 1 h, allowed to stand overnight at room temp., stirred with H2O at room temp., and treated with Dowex 50W .times. 8 (H+) to give 41% II (R = H). II (R = Me, Me2CH) were also prepd.
IC C07H007-06
CC 33-7 (Carbohydrates)
IT **67187-18-2P** 71972-01-5P 71972-02-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **67187-18-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 67187-18-2 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 18 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:517147 HCAPLUS
DOCUMENT NUMBER: 91:117147
TITLE: Adenosine analogs and human platelets. II. Inhibition of ADP-induced aggregation by carbocyclic adenosine and imidazole-ring modified analogs. Significance of alterations in the nucleotide pools
AUTHOR(S): Agarwal, Kailash C.; Parks, Robert E., Jr.; Townsend,

Leroy B.
CORPORATE SOURCE: Div. Biol. Med., Brown Univ., Providence, RI, USA
SOURCE: Biochem. Pharmacol. (1979), 28(4), 501-10
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Alterations in the ribose moiety of adenosine (I) [58-61-7] diminished the effectiveness in blocking platelet aggregation induced by 10.mu.M ADP [58-64-0]. Replacement of the 5'-OH of the ribose moiety by carboxyl, amino, or S-Me groups decreased the capacity to inhibit aggregation, but carbocyclic I (II) [19186-33-5], in which an O atom of the ribofuranosyl ring is replaced by a CH2 group, retained its full ability to inhibit ADP-induced aggregation. Modification of the imidazole portion of the purine ring of I had complex effects. No relation was established between I analog incorporation into platelet nucleotide pools, and their ability to inhibit ADP-induced aggregation. Thus, most of the I analogs examd. which inhibited platelet aggregation, probably did not function through formation of analog polyphosphate nucleotides or by alteration of the natural adenine nucleotide pools, and the possible actions of I and its analogs may be highly complex.

CC 1-3 (Pharmacodynamics)

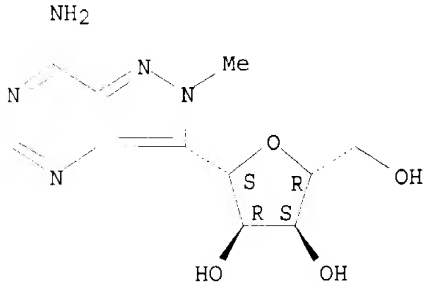
IT 69-33-0 606-58-6 2457-80-9 5682-25-7 6742-12-7 10299-44-2
14365-44-7 16136-63-3 18417-89-5 19186-33-5 20201-56-3
21193-80-6 24386-93-4 **42204-46-6** 51222-28-7 52326-94-0
53910-25-1 55559-56-3 57071-59-7 57071-61-1 59696-85-4
RL: BIOL (Biological study)
(platelet ADP-induced aggregation inhibition by, structure in relation to)

IT **42204-46-6**
RL: BIOL (Biological study)
(platelet ADP-induced aggregation inhibition by, structure in relation to)

RN 42204-46-6 HCAPLUS

CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

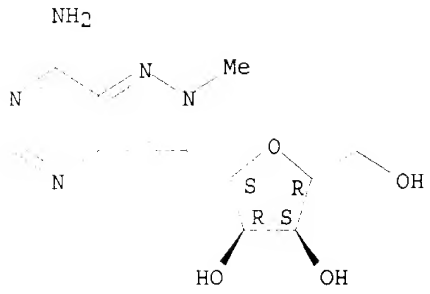
Absolute stereochemistry.



L5 ANSWER 19 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:415775 HCAPLUS
DOCUMENT NUMBER: 91:15775
TITLE: Adenosine kinase from rabbit liver. II. Substrate and inhibitor specificity
AUTHOR(S): Miller, Richard L.; Adamczyk, David L.; Miller, Wayne H.; Koszalka, George W.; Rideout, Janet L.; Beacham, Lowrie M., III; Chao, Esther Y.; Haggerty, Jerald J.;

Krenitsky, Thomas A.; Elion, Gertrude B.
CORPORATE SOURCE: Wellcome Res. Lab., Research Triangle Park, NC, 27709, USA
SOURCE: J. Biol. Chem. (1979), 254(7), 2346-52
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Kinetic consts. for substrates and inhibitors of highly purified rabbit liver adenosine kinase were detd. for 119 nucleosides and nucleoside analogs. The enzyme was relatively nonsp. with regard to the base moiety of ribonucleosides. The best substrates were adenosine, 8-azaadenosine, toyocamycin, and sangivamycin. Although imidazole ribonucleosides and some of their analogs served as substrates, their K'm values were >1000 times that of adenosine. None of the pyrimidine ribonucleosides tested were substrates or inhibitors. The enzyme was relatively specific for the ribosyl moiety. 2'-Deoxyadenosine and arabinosyladenine were extremely poor substrates, with substrate efficiencies of 10-4-10-6 that of adenosine. Binding of the inhibitor, 5'-deoxy-5'-aminoadenosine appeared to be pH-dependent. Basically, these results support the suggestion that a 2'-hydroxyl group trans to the glycoside linkage is a prerequisite for substrate activity or appreciable binding to the enzyme. A trans-2'-amino group was able to replace the 2'-hydroxyl group without loss of substrate activity. Studies with adenosine analogs locked in defined conformations suggest that binding to the enzyme does not appear to be solely dependent upon conformation.
CC 7-3 (Enzymes)
IT 58-61-7, reactions 58-63-9 69-33-0 73-03-0 146-77-0 146-78-1
146-92-9 342-69-8 524-69-6 550-33-4 606-58-6 958-09-8
1867-73-8 2096-10-8 2273-78-1 2504-55-4 2620-62-4 2946-39-6
3258-05-7 3414-62-8 3868-38-0 4229-57-6 4294-16-0 4338-47-0
5128-01-8 5399-87-1 5536-17-4 5746-29-2 6165-03-3 6742-12-7
7132-71-0 7724-76-7 10299-44-2 10414-81-0 13286-04-9 13351-68-3
14357-08-5 14675-48-0 15763-12-9 15824-83-6 16136-63-3
16220-07-8 18417-89-5 20125-39-7 23096-10-8 23589-16-4
26293-51-6 28542-78-1 29204-54-4 29851-57-8 30868-30-5
36791-04-5 41552-92-5 **42204-46-6** 51222-28-7 56964-77-3
58650-06-9 60355-67-1 62156-19-8 64372-74-3 70421-25-9
70421-26-0
RL: RCT (Reactant)
(reaction of, with adenosine kinase, kinetics of)
IT **42204-46-6**
RL: RCT (Reactant)
(reaction of, with adenosine kinase, kinetics of)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 20 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:444084 HCAPLUS
DOCUMENT NUMBER: 89:44084
TITLE: Cyclic phosphates of formycin
AUTHOR(S): Makabe, Osamu; Miyadera, Akihiko; Kinoshita, Mitsuhiro; Umezawa, Sumio; Takeuchi, Tomio
CORPORATE SOURCE: Fac. Eng., Keio Univ., Yokohama, Japan
SOURCE: J. Antibiot. (1978), 31(5), 456-67
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2',3'-Cyclic and 3',5'-cyclic phosphates of formycin and of N2-methyl- and N2-isopropylformycin were prepd. Thus, formycin was phosphorylated with Cl3CP(O)Cl2 in (EtO)3PO and the resultant formycin 5'-[(trichloromethyl)phosphonate] was hydrolyzed with Me3COK to give formycin 2,5'-cyclic phosphate. Methylation and ispropylation of formycin gave mixts. of N1-alkyl and N2-alkylformycins, which were sepd. and the latter were converted to the cyclic phosphates. Cyclic phosphorylation or N1- or N2-substitution with a bulky alkyl group made formycin resistant to deamination by adenosine deaminase. The cyclic phosphates were not effective as antitumor agents against L-1210 at 250 .mu.g/mouse/day.

CC 33-7 (Carbohydrates)
Section cross-reference(s): 1

IT **67187-21-7P** 67187-25-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzoylation of)

IT 67184-77-4P **67187-22-8P** 67187-26-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deisopropylidination of)

IT 22643-96-5P 54532-48-8P 67187-15-9P **67187-18-2P**
67187-20-6P **67187-24-0P** 67187-28-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymic deamination of)

IT 67187-14-8P **67187-17-1P** 67187-19-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

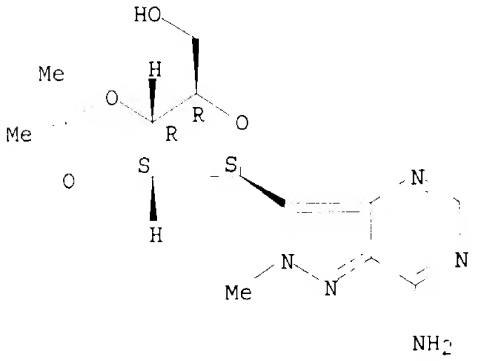
IT **42204-46-6P** 67184-74-1P 67187-16-0P **67187-23-9P**
67187-27-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphorylation of)

IT **67187-21-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzoylation of)

RN 67187-21-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-

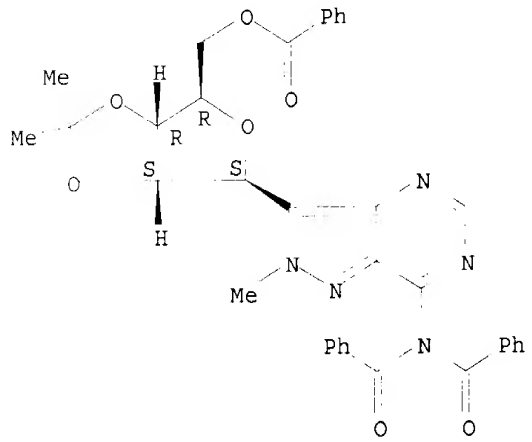
anhydro-2,3-O-(1-methylethylidene)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



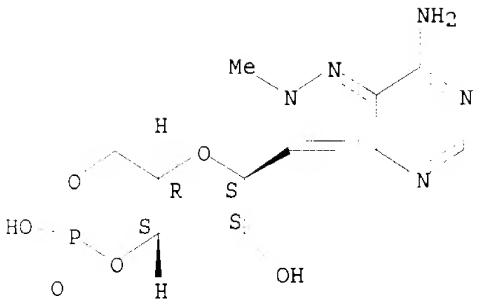
IT **67187-22-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deisopropylidination of)
RN 67187-22-8 HCAPLUS
CN Benzamide, N-benzoyl-N-[3 [5-O-benzoyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranosyl]-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



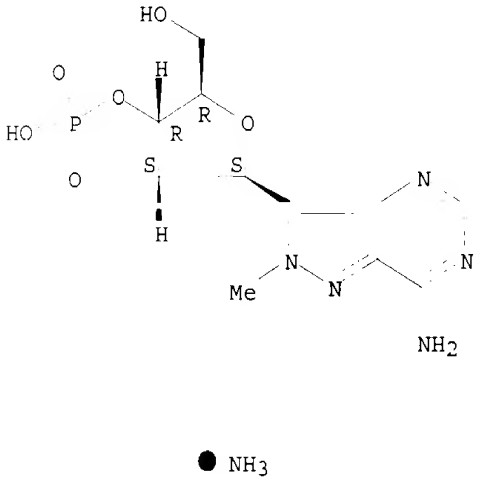
IT **67187-18-2P 67187-24-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymic deamination of)
RN 67187-18-2 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



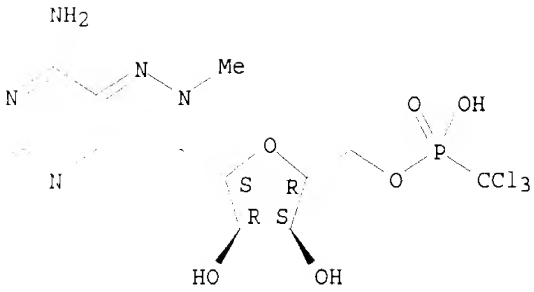
RN 67187-24-0 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 2,3-(hydrogen phosphate), monoammonium salt, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **67187-17-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 67187-17-1 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 5-[hydrogen (trichloromethyl)phosphonate], hydrochloride (2:1), (S)- (9CI) (CA INDEX NAME)

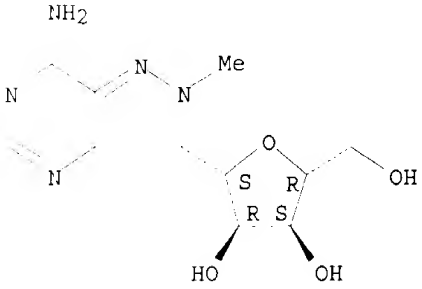
Absolute stereochemistry.



●1/2 HCl

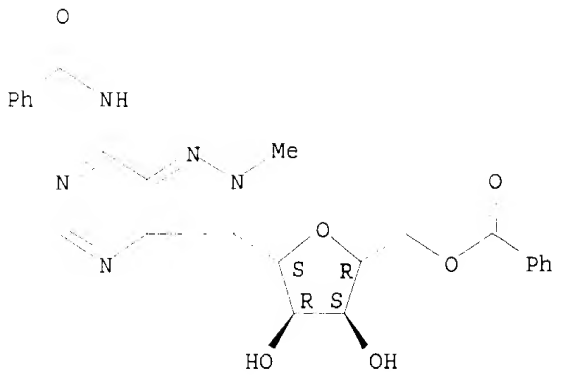
IT **42204-46-6P 67187-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphorylation of)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 67187-23-9 HCAPLUS
CN Benzamide, N-[3-(5-O-benzoyl-.beta.-D-ribofuranosyl)-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

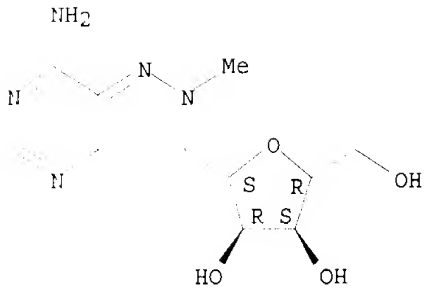


L5 ANSWER 21 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:38100 HCAPLUS
DOCUMENT NUMBER: 88:38100
TITLE: Preparation and properties of formycin analogs methylated on the pyrazolo ring nitrogens and/or the ribose cis-hydroxyls
AUTHOR(S): Giziewicz, Jerzy; Shugar, David
CORPORATE SOURCE: Inst. Biochem. Biophys., Pol. Acad. Sci., Warsaw, Pol.
SOURCE: Acta Biochim. Pol. (1977), 24(3), 231-46
CODEN: ABPLAF
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2'-O-Methyl, 3'-O-methyl, N1-methyl and N2-methyl derivs. of formycin A were prepd. by treatment with diazomethane in the presence or absence of SnCl2. Also prepd. were the 4 dimethylated derivs. Enzymatic deamination of N2-methylformycin A gave N2-methylformycin B. The active species in the SnCl2 catalyzed monomethylation of the 2'(3') cis hydroxyls of the ribonucleosides by CHN2 was an organotin product which contained no N or Cl. The sequence of elution of N1-methylformycin and N2-methylformycin on the strongly basic ion exchange column suggests that the latter is in the syn conformation, whereas the susceptibility of N2-methylformycin to adenosine deaminase shows that it may adopt the anti conformation on reaction with the enzyme.

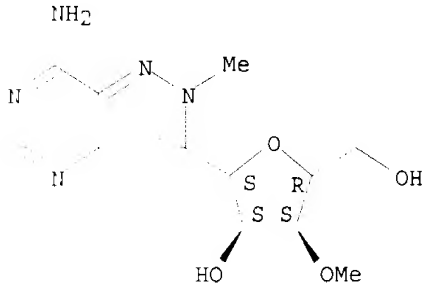
CC 33-7 (Carbohydrates)
Section cross-reference(s): 28
IT 6742-12-7DP, methylated **42204-46-6P** 51222-28-7P 58400-86-5P 58400-87-6P 65300-25-6P **65300-26-7P 65300-27-8P** 65300-28-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and UV spectra of)
IT **42204-46-6P 65300-26-7P 65300-27-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and UV spectra of)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



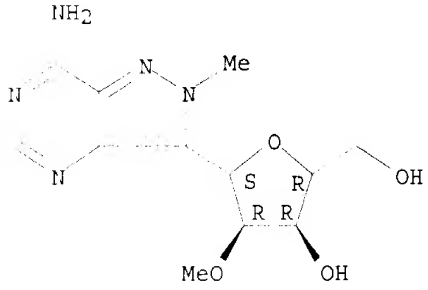
RN 65300-26-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-3-O-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 65300-27-8 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-2-O-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 22 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:543394 HCAPLUS
DOCUMENT NUMBER: 85:143394
TITLE: Carbon-13 magnetic resonance spectra of C-nucleosides. 3. Tautomerism in formycin and formycin B and certain pyrazolo[4,3-d]pyrimidines
AUTHOR(S): Chenon, Marie T.; Panzica, Raymond P.; Smith, James

C.; Pugmire, Ronald J.; Grant, David M.; Townsend, Leroy B.
CORPORATE SOURCE: Serv. Spectrochim. Infarouge Raman, CNRS, Thiais, Fr.
SOURCE: J. Am. Chem. Soc. (1976), 98(16), 4736-45
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Pyrazolo[4,3-d]pyrimidine heterocycles and nucleosides were examd. by C-13 NMR spectroscopy. The C chem. shifts and line widths of arom. and carbohydrate C were a function of temp. Through an anal. of the C chem. shift data, the tautomeric populations of the C-nucleosides formycin (I) and formycin B (II) were detd. The prototropic N(1)H .dblharw. N(2)H process which occurs in the pyrazole portion of the heterocyclic aglycon was the only tautomeric process obsd. in these nucleosides. The percentage of the N(2)H tautomer was dependent on the substituent at C-7 in the pyrazolo[4,3-d]pyrimidine ring.

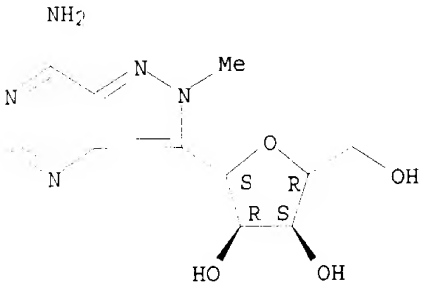
CC 33-7 (Carbohydrates)
Section cross-reference(s): 22, 28

IT 5399-94-0 6742-12-7 13264-01-2 13387-98-9 13877-55-9 13877-76-4
42204-46-6 51222-25-4 51222-26-5 51222-28-7
60753-31-3
RL: PRP (Properties)
(carbon-13 NMR of, tautomerism in relation to)

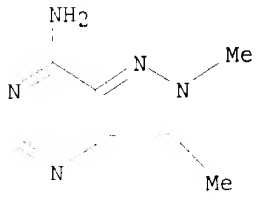
IT **42204-46-6 51222-25-4**
RL: PRP (Properties)
(carbon-13 NMR of, tautomerism in relation to)

RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 51222-25-4 HCAPLUS
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2,3-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 23 OF 27 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:99169 HCAPLUS
DOCUMENT NUMBEP: 84:99169
TITLE: Antiviral and antimetabolic activities of formycin and its N1-, N2-, 2'-O-, and 3'-O-methylated derivatives
AUTHOR(S): Giziewicz, J.; De Clercq, E.; Luczak, M.; Shugar, D.
CORPORATE SOURCE: Inst. Biochem. Biophys., Warsaw, Pol.
SOURCE: Biochem. Pharmacol. (1975), 24(19), 1813-17
CODEN: BCPCA6
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Formycin B [13877-76-4] and N1-methyl- [51222-28-7], 2'-O-methyl [58400-86-5], and 3'-O-methylformycin A [58400-87-6] were inactive against vaccinia, herpes simplex, and vesicular stomatitis viruses in primary rabbit kidney cells whereas formycin A [6742-12-7] inhibited the cytopathic effects of vaccinia at 10-40 .mu.g/ml and vesicular stomatitis virus at 2 .mu.g/ml. N2-methylformycin A (I) [**42204-46-6**] gave good activity against vaccinia virus and, unlike formycin A, was not toxic to the cells and did not affect cellular DNA and RNA synthesis at antiviral concns.

CC 1-4 (Pharmacodynamics)

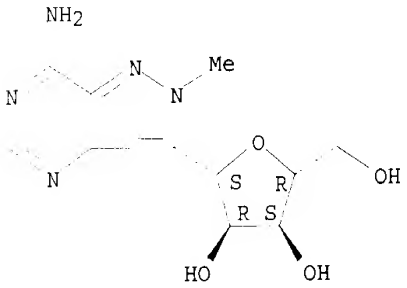
IT 6742-12-7 **42204-46-6**
RL: PRP (Properties)
(antiviral and antimetabolic effect of)

IT **42204-46-6**
RL: PRP (Properties)
(antiviral and antimetabolic effect of)

RN 42204-46-6 HCAPLUS

CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

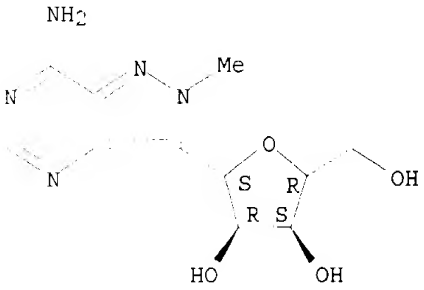
Absolute stereochemistry.



L5 ANSWER 24 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:527954 HCAPLUS
DOCUMENT NUMBER: 81:127954
TITLE: Molecular and crystal structures of 3-methylguanine, 8-ethyl-6-methyl-1,3,4-thiadiazolo[3-2a]-pyrimidine-5,7-dione, 2-methylformycin, and 8-chloroisoadenosine, chemotherapeutic derivatives of nucleic acid components. Automated deconvolution of the Patterson synthesis using superposition methods
AUTHOR(S): Abola, Jaime E.
CORPORATE SOURCE: Univ. Pittsburgh, Pittsburgh, Pa., USA
SOURCE: (1973) 210 pp. Avail.: Univ. Microfilms, Ann Arbor, Mich., Order No. 74-18,422
From: Diss. Abstr. Int. B 1974, 35(2), 990

DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
CC 70-5 (Crystallization and Crystal Structure)
IT 2958-98-7 34408-11-2 **42204-46-6** 53799-00-1
RL: PRP (Properties)
(crystal structure of)
IT **42204-46-6**
RL: PRP (Properties)
(crystal structure of)
RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



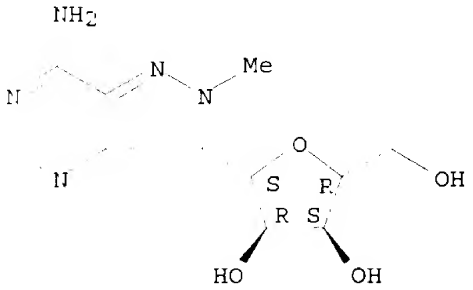
L5 ANSWER 25 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:478181 HCAPLUS
DOCUMENT NUMBER: 81:78181
TITLE: Pyrazolopyrimidine nucleosides. V. Methylation of the C-nucleoside antibiotic formycin and structural elucidation of products by magnetic circular dichroism spectroscopy
AUTHOR(S): Townsend, Leroy B.; Long, Robert A.; McGraw, James P.; Miles, Daniel W.; Robins, Roland K.; Eyring, Henry
CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, Utah, USA
SOURCE: J. Org. Chem. (1974), 39(14), 2023-7
CODEN: JOCEAH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The direct methylation of formycin gave 7-amino-1-methyl-3-.beta.-D-ribofuranosylpyrazolo[4,3-d]pyrimidine (I) and 7-amino-2-methyl-3-.beta.-D-ribofuranosylpyrazolo[4,3-d]-pyrimidine (II). The above structures were detd. by a comparison of the magnetic circular dichroism (MCD) curves obtained for the model compds. 7-amino-2,3-dimethylpyrazolo-[4,3-d]pyrimidine (III) and 7-amino-1,3-dimethylpyrazolo [4,3-d]-pyrimidine (IV) with the MCD spectra of I and II. Ring annulation of the appropriately substituted pyrazole precursors gave III and IV. The synthesis of 1,3-dimethylpyrazolo[4,3-d]pyrimidin-7-one and 2-methyl-3-.beta.-D-ribofuranosylpyrazolo[4,3-d]pyrimidin-7-one was accomplished by an unusual displacement of the exocyclic amino group in 1N NaOH.
CC 33-7 (Carbohydrates)
Section cross-reference(s): 28
IT 32183-14-5P **42204-46-6P** 51222-23-2P 51222-24-3P
51222-25-4P 51222-26-5P 51222-27-6P 51222-28-7P

51481-59-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

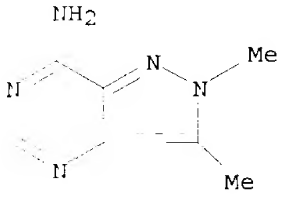
IT **42204-46-6P 51222-25-4P 51481-59-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

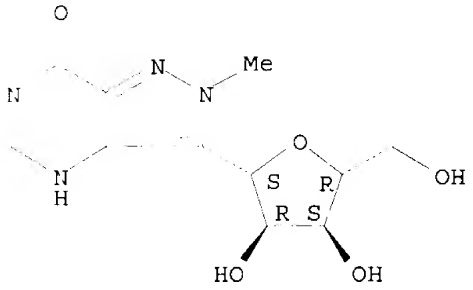


RN 51222-25-4 HCAPLUS
CN 2H-Pyrazolo[4,3-d]pyrimidin-7-amine, 2,3-dimethyl- (9CI) (CA INDEX NAME)



RN 51481-59-5 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-2-methyl-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 26 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:421792 HCAPLUS

DOCUMENT NUMBER: 81:21792
TITLE: Molecular structure and conformation of the nucleoside antibiotic derivative 2-methylformycin with a C-glycosidic bond
AUTHOR(S): Abola, Jaime E.; Sims, Michael J.; Abraham, Donald J.; Lewis, Arthur F.; Townsend, Leroy B.
CORPORATE SOURCE: Dep. Med. Chem., Univ. Pittsburgh, Pittsburgh, Pa., USA
SOURCE: J. Med. Chem. (1974), 17(1), 62-5
CODEN: JMCMAR
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The mol. and crystal structure of 2-methylformycin (I) [**42204-46-6**] as detd. by x-ray techniques gave the space group as monoclinic P21, and cell dimensions as a = 9.208, b = 14.367, and c = 4.791 .ang., and .beta. = 101.9.deg.. The conformation about the C-glycosidic bond is syn and about the hydroxymethylene group on the ribose is gauche-gauche. The relation between conformation and antileukemic activity is discussed.

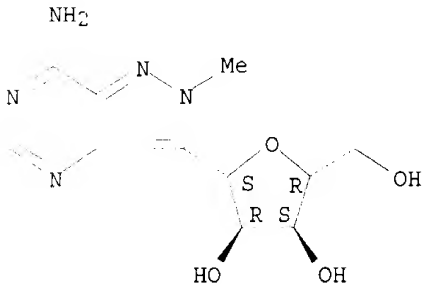
CC 3-13 (Biochemical Interactions)
Section cross-reference(s): 28, 33, 70

IT **42204-46-6**
PL: PRP (Properties)
(mol. structure and conformation of, antileukemic activity in relation to)

IT **42204-46-6**
PL: PRP (Properties)
(mol. structure and conformation of, antileukemic activity in relation to)

RN 42204-46-6 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 27 OF 27 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:413415 HCAPLUS
DOCUMENT NUMBER: 79:13415
TITLE: Inhibitors of purine metabolism in Ehrlich ascites tumor cells in vitro
AUTHOR(S): Lau, K. F.; Henderson, J. Frank
CORPORATE SOURCE: Cancer Res. Unit, Univ. Alberta, Edmonton, Alberta, Can.
SOURCE: Cancer Chemother. Rep., Part 2 (1973), 3(1), 95-109
CODEN: CCSUBJ
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Of 92 purine analogs and derivs. tested for their ability to inhibit 8 enzymes of purine metab. as well as for their effect on the ratios of ATP/(ADP + AMP) and GTP/(GDP + GMP) in Ehrlich ascites tumor cells in vitro, 52 compds. were inhibitory to at least 1 system, and 25, including 6-(cyclopentylthio)-9H-purine-9-methanol (I) [14196-96-4], were inhibitory in 2 or more systems.

CC 1-4 (Pharmacodynamics)

IT 50-44-2 69-33-0 85-31-4 146-78-1 524-69-6 550-33-4 574-25-4
958-09-8 1818-71-9 1867-73-8 2004-04-8 2096-10-8 2104-65-6
2500-80-3 2504-55-4 2946-39-6 3080-29-3 3414-62-8 3969-27-5
4005-33-8 4294-16-0 4338-48-1 4857-06-1 4921-56-6 5399-87-1
5470-25-7 5536-17-4 5746-27-0 5746-29-2 6273-05-8 6742-12-7
6974-67-0 7252-00-8 7724-76-7 7803-88-5 10279-87-5 10299-44-2
10310-21-1 11033-22-0 13083-37-9 13389-08-7 13389-16-7
14196-95-3 14196-96-4 14426-53-0 15397-51-0 15717-47-2
15717-48-3 16033-27-5 17434-50-3 19792-96-2 20187-89-7
20350-17-8 20371-00-0 20419-68-5 20789-67-7 22387-37-7
22415-88-9 24386-90-1 24386-91-2 24386-93-4 25253-77-4
26315-51-5 27963-76-4 28069-17-2 33585-52-3 40089-75-6
40297-52-7 42204-07-9 42204-09-1 42204-10-4 42204-26-2
42204-29-5 42204-31-9 42204-34-2 42204-35-3 42204-36-4
42204-37-5 42204-38-6 42204-39-7 42204-40-0 42204-41-1
42204-42-2 42204-43-3 42204-44-4 **42204-46-6** 42204-47-7
42311-25-1

PL BIOL (Biological study)
(purine metab. by neoplasm in response to)

IT **42204-46-6**

PL BIOL (Biological study)
(purine metab. by neoplasm in response to)

RN 42204-46-6 REGISTRY

CN D-Ribitol, 1-C-(7-amino-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.